

Topological pumps and adiabatic cycles

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Topological insulators have gapless states at their boundaries while trivial insulators generically do not. We consider loops in the spaces of Hamiltonians of topologically trivial Bloch insulators, and show that there exist loops for which the boundary gap must necessarily close at some point or points along the loop. We show that some of these loops may be regarded, depending on the symmetry class of the insulator and its physical dimension, as defining pumps of charge, fermion parity, and in more exotic cases of other quantities such as a Z_2 parity.

It has recently been recognized that ordinary Bloch insulators with time-reversal symmetry (TRS) come in more than one variety [1–4]. Since the first predictions and the subsequent experimental confirmations, the field of topological insulators (Bloch insulators of the non-trivial variety) has seen an explosion of both theoretical and experimental interest [5]. Topological insulators belong to a different phase of Bloch insulators than trivial insulators and it is impossible to go continuously from the Hamiltonian of a trivial insulator to that of a topological insulator without going through a point where the bulk gap closes. Thus, the existence of topological insulators for a particular symmetry class and physical dimension reveals an interesting fact about the topological structure of the corresponding space of Bloch Hamiltonians, namely that there are paths in this space along which the bulk gap must necessarily close at some point or points.

In this paper, we consider a related issue which is the following: Are there loops in the space of Bloch Hamiltonians of trivial insulators (which generically do not have gapless boundary states) along which the boundary gap (in a system with a boundary) necessarily closes at some point or points despite the bulk gap staying open throughout the loop? A loop in the space of Bloch Hamiltonians for which the bulk excitation gap remains open may be regarded as an adiabatic cycle of a Bloch insulator, a term we use to describe the process of transforming gradually the Hamiltonian of a Bloch insulator by changing, for instance, the periodic potential. Physically, one can imagine an adiabatic cycle arising from a continuous and periodic physical perturbation such as a strain that leads to a distortion of the periodic potential and hence the band structure. We call adiabatic cycles for which the boundary gap must necessarily close non-trivial adiabatic cycles. Later, we will argue that there is indeed a non-trivial topological structure to these loops and that they may be assigned a non-trivial “bulk” topological invariant which may be determined from the bulk wavefunctions when periodic boundary conditions are used.

We will see that, though not originally studied from the perspective of a closing of the boundary gap in a finite system, the charge pumps in one dimension (1d) introduced by Thouless [6] are examples of non-trivial

adiabatic cycles in the sense discussed above, i.e., they are accompanied by a closing of the boundary gap in a semi-infinite system with an boundary. In the case of the Thouless charge pump, we shall see that the total fermion number or charge of the ground state in a semi-infinite system changes along with a closing of the gap. For a 1d system with two boundaries, this leads to the picture of charge entering through one boundary and leaving through the other in the course of a cycle. Thus, the adiabatic cycle may be regarded as a pumping of charge. A similar process occurs for some other classes of non-trivial adiabatic cycles that we study. In some of these cases, quantum numbers such as a Hall conductance, or spin Hall conductance may be associated with the states that cross the Fermi energy. Thus the corresponding adiabatic cycles may be regarded as “Hall pumps” or “spin Hall” pumps.

The remainder of the paper is organized as follows. We first provide a topological classification of adiabatic cycles based on their bulk Bloch wavefunctions using known results of K-theory. We then go on to argue that adiabatic cycles with a non-trivial bulk topological invariant lead to a closing of the gap in systems with an boundary. Thereafter, we discuss a number of interesting examples of topological adiabatic cycles and their boundary invariants and pumping properties.

We begin with a topological classification of adiabatic cycles. Our primary interest is in the case of insulators belonging to the trivial class. Since, however, it is no harder to do so, we will also consider cases where the insulators are topologically non-trivial. The classification of adiabatic cycles is based on questions similar to those that led to a classification of insulators. Are there adiabatic cycles which cannot be deformed into each other by a continuous deformation of the band structure? It is clear that quantities such as the number of occupied bands of a band insulator and its topological class are invariants of an adiabatic cycle. A complete classification of all such invariants can be obtained using the tools of K-theory which have recently led to a fuller understanding of the periodic structure in the classification of topological insulators [7]. Our focus is primarily on a particular class of invariants of the adiabatic cycles, which we call

the strong invariants. There is a chain in dimensions in the structure of the topological invariants. Invariants associated with adiabatic cycles of d -dimensional insulators always lead to invariants of adiabatic cycles of $d+1$ -dimensional insulators. This situation is reminiscent of topological insulators in 3d, where there are 4 invariants, three of which may be thought of as 2d or “weak” invariants, and one of them is an intrinsically 3d or “strong” invariant. In the current situation, both the topological invariant of the insulator as well as the lower dimensional invariants of the adiabatic cycles can be regarded as weak invariants.

We now explicitly identify a group associated with the strong invariants of adiabatic cycles of Bloch insulators without TRS. In the tight-binding representation, the Hamiltonian for electrons in a periodic potential can be represented by a Hermitian matrix at each point in the Brillouin zone. Setting the chemical potential to zero, this matrix has non-vanishing determinant in a Bloch insulator. The Brillouin zone for a d -dimensional insulator is topologically equivalent to the d -torus, T^d and a loop, to the unit circle, S^1 . Thus, an adiabatic cycle defines a smooth map from $T^d \times S^1$ to the set, $\mathcal{H}(d, 1)$, of Hermitian matrices which have non-zero determinant. An equivalence relation can be defined for these maps which isolates the strong topological invariant of the adiabatic cycles in much the same way as in the case of topological insulators [7]. Further, we can define an operation which, given two maps, H_1, H_2 from $T^d \times S^1$ to $\mathcal{H}(d, 1)$, produces a third map whose value at a given point (k, t) in $T^d \times S^1$ is the direct sum, $H_1(k, t) \oplus H_2(k, t)$, of the matrices, $H_1(k, t), H_2(k, t)$ obtained from the two maps, H_1 and H_2 . The set of the equivalence classes of maps defined through the equivalence relation mentioned earlier forms a group, G , under this operation, which is in fact isomorphic to a group denoted by $\tilde{K}(S^{d+1})$ in K-theory. It is a standard result in K-theory that this group is the set of integers for odd d and the trivial group for even d [8].

The symmetries of the insulator play a crucial part in the classification of their adiabatic cycles by imposing constraints on the corresponding maps from $T^d \times S^1$ to $\mathcal{H}(d, 1)$. Each fundamental set of symmetries (such as TRS and particle-hole symmetry) of an insulator corresponds to one of the ten Altland Zirnbauer (AZ) symmetry classes of random matrices [9]. Using the constraints imposed by symmetries and the procedure outlined above, one can identify the appropriate K groups for the classification of the strong invariants of adiabatic cycles in all the AZ symmetry classes with the help of standard results in K-theory [8, 10]. This is analogous to the classification of topological insulators and defects using K-theory which has been outlined in several recent works [7, 11, 12]. The results of the classification are presented in Table I.

We now relate the existence of distinct equivalence

TABLE I. Classification of adiabatic cycles of Bloch insulators. Each column corresponds to a particular symmetry class identified by its Cartan label with the different rows corresponding to different physical dimensions.

d	A	AIII	AI	BDI	D	DIII	AII	CII	C	CI
0	0	Z	Z_2	Z_2	0	Z	0	0	0	Z
1	Z	0	Z	Z_2	Z_2	0	Z	0	0	0
2	0	Z	0	Z	Z_2	Z_2	0	Z	0	0
3	Z	0	0	0	Z	Z_2	Z_2	0	Z	0

classes of adiabatic cycles to the closing of the boundary gap. Consider an infinite d -dimensional ($d \geq 1$) trivial insulator which we regard as two semi-infinite insulators, labeled left and right, joined at the $d-1$ dimensional plane, $x = 0$. Let us now imagine that we smoothly change the Hamiltonian of the left insulator as a function of a parameter, t , along the path of a non-trivial topological adiabatic cycle while the Hamiltonian of the right is kept constant. At $t = 0$, the Hamiltonian is the same for the left and the right insulators. For small t , one can expect to vary the Hamiltonian in the vicinity of $x = 0$ without forming localized sub-gap states in the vicinity of this plane. However, it is clear that this can not be done for all t . Indeed, if it could, it would define a continuous deformation from the adiabatic cycle on the left to the constant or trivial loop on the right. Since the cycle on the right is a topological adiabatic cycle, and, by definition, one which cannot be continuously deformed to a constant one, this provides a contradiction, thus proving the existence of gapless boundary states. These boundary modes are expected to persist when one replaces the trivial insulator with the vacuum.

d=1: Let us now study the simplest examples of non-trivial adiabatic cycles which are accompanied by a closing of the boundary gap, namely the charge pumps of 1d insulators without TRS, which were studied by Thouless in the context of quantized fermion number transport [6]. Consider a semi-infinite 1d insulator which extends along the positive x-axis, whose Hamiltonian, $H_{1d}(t)$, is varied along the path of a topological adiabatic cycle such that $H_{1d}(2\pi) = H_{1d}(0)$. This cycle can be mapped onto the Hamiltonian, H_{2d} , of a 2d Bloch insulator on a cylinder, by writing $H_{2d} = \sum_{k_y} H_{1d}(t = k_y)$, where k_y is the scaled momentum along the circumference of the cylinder. From the defining property of a 1d charge pump, the 2d Bloch insulator displays the integer quantum Hall effect. Consequently, it must have boundary modes on account of Laughlin’s gauge argument [13] and so must the adiabatic cycle. Let $\{t_i\}$ be the set of points at which gapless zero energy states occur. In the vicinity of these points, one may define boundary Hamiltonians, $H_b(t) = \sum_i E_i |u_i(t)\rangle\langle u_i(t)|$, where the sum is over all states that decay exponentially away from the bound-

ary. One can always ensure (through slight deformations of the Hamiltonian, if necessary) that there exists some interval, $[t_i - \epsilon, t_i + \epsilon]$, around each of the t_i such that no extended states join the set of localized boundary states in this interval and that the boundary Hamiltonian has a gap (albeit small) at the end points of the interval.

Let n_i^\pm be the charges associated with the ground states of the boundary Hamiltonians, $H_b(t_i \pm \epsilon)$. Then, the net spectral flow associated with the cycle is equal to $\sum_i n_i^+ - \sum_i n_i^-$. It cannot change by arbitrary deformations of the boundary spectrum and is hence an invariant of the cycle. Using Laughlin's gauge argument (which proves the correspondence between the Chern invariant and spectral flow for the 2d Bloch insulator) and the correspondence between the 1d and the 2d systems, it is easy to prove that this boundary invariant must equal the bulk topological invariant of the adiabatic cycle. The flow at the gapless points in the boundary spectrum leads to a flow of fermions from the occupied states to the unoccupied states in a system with a fixed number of particles. (In a system with a fixed chemical potential, it leads to a flow of particles in and out of the system.) Thus the adiabatic cycle can be regarded as a fermionic number pump, or a charge pump for a system with charged fermions.

Adiabatic cycles of 1d insulators in classes AI and AII are also classified by an integer (\mathbb{Z}) invariant. In both of these cases, the first Chern number provides the topological invariant, and there is a net spectral flow and consequently a pump of fermion number. Time-reversal symmetry ensures that the net fermion number pumped in the case of Class AII is always an even integer.

Further interesting cases are the Z_2 adiabatic cycles of insulators in classes BDI and D. Consider a topological adiabatic cycle of a semi-infinite 1d trivial superconductor. If at a degeneracy point, t_0 , a single pair of boundary states crosses zero, the parity of the ground state changes [14]. The net change in parity across all the gapless points is an invariant of the cycle and is non-trivial for a cycle with a non-trivial Z_2 invariant, E . The fermion parity pump studied above is qualitatively different from the Josephson junction of a 1d topological superconductor studied before [12, 15] where no spectral flow occurs when open boundary conditions are used.

d=2: We next consider insulators in two spatial dimensions and argue that the non-trivial cycles in classes D and DIII and those characterized by an odd integer in class BDI can be regarded as parity pumps. Let us first examine adiabatic cycles of insulators in Class D. Consider a 2d crystal with lattice basis vectors ($\mathbf{a} = a\hat{y}, \mathbf{b}$) which has periodic boundary conditions and an even number of unit cells in the y -direction (for convenience of discussion) and is semi-infinite along \mathbf{b} . At each point of time, t , the Hamiltonian can be written as a sum: $\mathcal{H}(t) = H(0, t) + H(\pi, t) + \sum_{0 < k_y < \pi} (H(k_y, t) + H(-k_y, t))$ where $0, \pi, k_y$ are the crystal momenta in the y -direction, rescaled so that they lie between $-\pi$ and π . Under

a particle-hole transformation, a general crystal momentum k_y goes to $-k_y$, while the momenta 0 and π are invariant. Thus, the operators $H(0, t), H(\pi, t)$ and $H'(k_y, t) = H(k_y, t) + H(-k_y, t)$ for $0 < k_y < \pi$ can all be regarded as defining adiabatic cycles of 1d superconducting Hamiltonians in class D and one may therefore associate Z_2 invariants, $E(0), E(\pi)$, and $E(k_y)$ with them. It is clear that $E(k_y)$ for $0 < k_y < \pi$ is always the trivial element of the group Z_2 . The topological invariant of an adiabatic cycle of a 2d superconductor is the product of the topological invariants $E(0)E(\pi)$. Since the net change in parity for the Hamiltonians, $H'(k_y)$, is always trivial, this product also determines the net change through spectral flow of the parity of a lattice superconductor with an even number of unit cells around the cylinder. A more general statement which is independent of the width of the cylinder is that the product of the net changes in parity for an adiabatic cycle in the presence and absence of a π flux along the axis of the cylinder is equal to the Z_2 invariant. Thus the non-trivial adiabatic cycles for 2d insulators in class D can be interpreted as parity pumps. From similar considerations, it is easy to show that the adiabatic cycles in class BDI with a topological invariant ν such that $|\nu|$ is an odd integer also correspond to parity pumps.

Non-trivial adiabatic cycles in class DIII in 2d can be regarded as spin or Z_2 parity pumps. For these pumps, one can write the ground state at any given moment as a product $|\Omega_I(t)\rangle|\Omega_{II}(t)\rangle$ where $|\Omega_I(t)\rangle$ gets mapped onto $|\Omega_{II}(t)\rangle$ under time-reversal symmetry. One can then define the associated parities, $P_I(t), P_{II}(t)$, such that the total parity is $P(t) = P_I(t)P_{II}(t)$ and while the net change in the parity of the entire system during the cycle is zero, there is a net change in the parities, $P_I(t)$ and $P_{II}(t)$ for non-trivial adiabatic cycles of insulators with an even number of unit cells in the periodic direction.

d=3: Similar arguments to those used above can be used to prove that adiabatic cycles of superconductors in 3d in class D with a “strong” 3d invariant $\nu \in \mathbb{Z}$ such that ν is odd can be regarded as parity pumps. Similarly, Z_2 adiabatic cycles of superconductors in class DIII with a non-trivial strong Z_2 invariant can be regarded as Z_2 parity pumps. In these cases, the net parity change occurs in systems with periodic boundary conditions and an even number of unit cells along two of the lattice basis vectors \mathbf{a}, \mathbf{b} and open boundary conditions along a third basis vector, \mathbf{c} . Again, a more general statements which covers the cases where there an odd number of unit cells in the periodic directions relates the topological invariant to the product of the net parity changes in the presence and absence of a π flux through each of the holes of the system with periodic boundary conditions.

Adiabatic cycles of insulators in 3d in class A (without TRS or any sub-lattice symmetry) are classified by a \mathbb{Z} invariant. We consider a particular non-trivial adiabatic cycle in a system which is periodic in the x, y directions

and semi-infinite in the z -direction, which has the feature that at $t = \pi$, the Hamiltonian corresponds to that of a strong topological insulator [10]. For $\tilde{t} = t - \pi$ close to 0, a low-energy effective continuum theory can be obtained by a Taylor expansion of the Hamiltonian around the point at which the gap closes, which in this case happens at $\mathbf{k} = (0, 0, 0)$ and $\tilde{t} = 0$. One can then analytically solve for the boundary state spectrum and obtain an boundary Hamiltonian, as outlined for the 1d case. On doing this, we obtain a 2D Dirac boundary Hamiltonian of the form:

$$H_b(\tilde{t}) = \int dk \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}^T \begin{pmatrix} \tilde{t} & -k_x + ik_y \\ -k_x - ik_y & -\tilde{t} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Now let us consider the same adiabatic cycle, but in the presence of a constant magnetic field, $\mathbf{B} = (0, 0, -B)$ where $B > 0$. It is well known that for a 2d Dirac Hamiltonian, in the presence of a magnetic field, relativistic Landau levels are formed [16]. The lowest Landau level has an energy, $\lambda_0 = \tilde{t}$ with a degeneracy of eB/h states per unit area. We see that, as \tilde{t} increases, this lowest Landau level crosses zero from below at $\tilde{t} = 0$.

For a finite system, we may associate a Hall conductance with the surface state whose energy crosses zero by computing the Chern number in the space of eigenvalues of the magnetic translation operators. Since the states that cross the Fermi energy (which is set at 0) have an associated Hall conductance, we regard non-trivial topological adiabatic cycles of 3d insulators as defining adiabatic pumps of Hall conductance. If we consider a cycle, where the system at the start of the cycle is a strong 3d topological insulator with a surface which has an boundary gap induced by a TRS breaking surface perturbation, then the surface Hall conductance at the end of a cycle in the presence of a magnetic field, while remaining a half integer, changes by an integer amount.

Non-trivial adiabatic cycles of superconductors in class C are classified by a Z invariant. These superconductors have an $SU(2)$ gauge symmetry associated with spin-rotational symmetry. Given a lattice Hamiltonian in this class of the form: $H = \sum_{s_3, i, j} t_{i, j, s_3} a_{i, s_3}^\dagger a_{j, s_3} + (\sum_{i, j} \Delta_{ij} a_{i, \uparrow}^\dagger a_{j, \downarrow}^\dagger + \text{h.c.})$ where orbital indices have been suppressed, i, j are site indices and $s_3 = 1, s_3 = -1$ correspond to up-spins and down-spins respectively, we consider an associated Hamiltonian obtained by a generalized Peierls substitution $t_{i, j, s_3} \rightarrow t_{i, j, s_3} e^{-is_3 \frac{e}{\hbar} (f_i^j \mathbf{A} \cdot d\mathbf{r})}$, $\Delta_{ij} \rightarrow \Delta_{ij} e^{-i \frac{e}{\hbar} (f_i^j \mathbf{A} \cdot d\mathbf{r})}$. Here, \mathbf{A} is the vector potential which corresponds to an uniform and commensurate magnetic field, \mathbf{B} in the z -direction. The resulting Hamiltonian can be considered to be that of the system in a fictitious $SU(2)$ gauge field. Even in the presence of the $SU(2)$ gauge, the Hamiltonian has a residual $U(1)$ symmetry for spin rotations about the z -axis. The states that cross the zero of energy at a point where the gap at the boundary vanishes can thus be assigned a Hall con-

ductance for spin along the z -direction. These adiabatic cycles can be therefore be interpreted as spin Hall pumps in the presence of an $SU(2)$ spin field.

Adiabatic cycles of 0d systems can not be regarded as pumps. However, we note that the Berry phase associated with adiabatic cycles in classes AI and BDI can only be 0 or π and the latter correspond to the non-trivial adiabatic cycles. Similarly, the adiabatic cycles of insulators in classes AIII and C with an odd integer invariant also have a Berry phase of π . This concludes our survey of some of the interesting examples of non-trivial adiabatic cycles. The current discussion did not cover adiabatic cycles in classes AIII, CII and CI, and those of 3d insulators in class AII which will be discussed elsewhere [10].

To summarize, we have studied the classification of adiabatic cycles of Bloch insulators. We showed that there exist non-trivial adiabatic cycles of trivial insulators, i.e., paths in the spaces of Bloch Hamiltonians where the boundary gap must necessarily close though the bulk gap remains open and the insulators are themselves in the trivial class. We found that many of these adiabatic cycles can be regarded as pumps and that the net change in certain quantum numbers associated with the states that cross the gap equals the topological invariant describing the cycles.

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